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EDITORIAL REPORT ON NOMENCLATURE, 1950.*

It is hoped to publish annually an Editorial Report on developments in nomenclature as practised in the Chemical Society's publications, to include broad questions of general principle and individual items of wide interest, but not matters of concern only in particular cases. In this, the first of such Reports, reliance has been placed on A. D. Mitchell's " British Chemical Nomenclature " (Edward Arnold, 1948) as giving standard British practice at the time of its publication (though the opinions expressed there on controversial matters have the weight of the author's long experience rather than of official rulings). The Reports will not necessarily be confined only to the previous twelve months; the present Report necessarily draws to some extent on earlier years to bridge the gap back to Dr. Mitchell's book, and it deals with matters of two types: (i) new decisions on nomenclature, and (ii) points of established nomenclature which warrant special mention.

At the outset it will be well to make clear two principles. First, strict systematic nomenclature need not be used in the Society's publications when it obscures genetic principles discussed in a particular paper. Acceptable variants can usually be found, but in such cases the systematic name should also be given at least once (usually best in the Experimental section) so that searchers can locate the substance in indexes; however, a real warrant is required for such exceptions. Secondly, those who hope for an invariable nomenclature are doomed to disappointment; nomenclature must develop as chemistry develops, and its value is proportional to its flexibility, particularly when new ideas require expression.

Inorganic.

Use of the names of elements recommended by the International Union of Pure and Applied Chemistry (Report of the 15th Conference, Amsterdam, 1949, p. 58) was approved by the Council of the Chemical Society, except that the name " tungsten " will not be replaced by " wolfram " (*Proc.*, 1950, 69; *J.*, 1951, 2). It may be noted that niobium (not columbium) is accepted (cf. *J.*, 1949, S223, 2472).

The paper on " Inorganic Chemical Nomenclature " by Ewens and Bassett (*Chem. and Ind.*, 1949, 131) was considered by the Publication Committee, but action has been deferred until the outcome of international deliberations is known (cf. 15th Report, etc., p. 58).

The names di-, tri-, and tetra-sulphuric acid have proved convenient for $H_2S_2O_7$ (pyrosulphuric), $H_2S_3O_{10}$, and $H_2S_4O_{13}$, respectively (*J.*, 1950, 2493 †); they are analogous to tetraboric acid $H_2B_4O_7$.

Organic.

Prefixes.—The alphabetical order of substituents denoted by prefixes has been made standard during 1950. The following details are given for reference.

The order is governed by the following principles, which follow in general those adopted in *Chemical Abstracts* except for differences in nomenclature, spelling, italicising, or punctuation. In these last respects current practice in the *Journal* is not affected.

Clarendon (black) type is used below to indicate alphabetical order; it is, of course, not used for this purpose in ordinary publications.

(*a*) The names of substituents cited as prefixes are arranged alphabetically, regardless of the number of each, as in:

o-**bromochlorobenzene**
8-nitro-1 : 2-diphenylquinoline
3-amino-4-nitro-2-naphthol
ethylmethylphenylcarbinol

* Reprints of this Report may be obtained from the General Secretary, The Chemical Society, price 1*s.*, post free.

† References to the *Journal*, here and elsewhere, are illustrative, not exhaustive.

(*b*) A compound radical name is treated as a unit. Thus "methylamino" is arranged under m, "dimethylamino" under d, "3-amino-4-nitro-2-naphthyl" under a. Cf.:

2-chloro-3-dimethylamino-4-hydroxypyridine
2-(3 : 5-dinitrophenyl)-3-ethylnaphthalene
2-(3 : 5-dinitrophenyl)-3-nitronaphthalene

(*c*) The above two rules may be combined as in:

3-chloro-1 : 4-bisdimethylamino-3-ethylnaphthalene
2-chloro-3-ethyl-1 : 4-bismethylaminonaphthalene

(*d*) Within a compound radical name, the alphabetical order is applied, when necessary, as in:

2-(4-ethyl-3 : 5-dinitrophenyl)furan [or 4-ethyl-1-2'-furyl-3 : 5-dinitrobenzene]
2-chloro-3-(4-ethyl-2-nitrophenyl)-1-methylnaphthalene

(*e*) Ordinary indexing rules are used; *e.g.*, short names precede longer ones with a similar beginning (methyl before methylamino, chloro before chlorophenyl, etc.), as in:

2-methyl-1-methylaminonaphthalene
1 : 1 : 1-trichloro-2 : 2-di-(*p*-chlorophenyl)ethane

(*f*) "Hydro" prefixes are arranged as beginning with h, although they do not, strictly speaking, denote substituents; *e.g.*,

1-ethyl-1 : 4-dihydro-4-methylnaphthalene

(*g*) All atoms or rings forming part of the fundamental chain or ring system are written as part of the fundamental name and are not movable (the alphabetical order applies only to substituents and to the addition of hydrogen); *e.g.*,

8-nitro-3 : 4-benz-2-quinolyl (not 3 : 4-benz-8-nitro-2-quinolyl)
1 : 2-3 : 4-dibenzanthraquinon-6-yl (under d)
3-nitroindolo(1' : 2'-1 : 2)quinoline (indolo is not a substituent)
3 : 6 : 9-triazaundecane (the system C_2–N–C_2–N–C_2–N–C_2 is indivisible)

(*h*) Similarly, the customary order of citation of hetero-atoms in rings or chains is unaffected; *e.g.*,

1 : 3 : 4-oxadiazole (not 3 : 4 : 1-diazaoxole)

(*i*) Syllables which indicate a change other than substitution are not detachable. Examples are 2-deoxyglucose (removal of oxygen), de-*N*-methylthebainone (removal of methyl), dehydrocholesterol (*removal* of hydrogen; contrast rule *f* above).

(*j*) In names consisting of more than one word separated by a space, the order laid down by the rules of nomenclature is unaffected; in other cases the order is alphabetical in such cases also; *e.g.*,

ethyl methyl adipate
methyl hydrogen phthalate
ethyl phenyl ketone
4-amino-3-chlorophenyl butyl ether
5 : 6-*iso*propylidene 3-toluene-*p*-sulphonyl α-methyl-D-glucoside

(*k*) Italicised prefixes are neglected when assembling substituents; but isomeric substituents are arranged in alphabetical order of the italicised prefixes, except that *iso* follows directly after *n*, and *o*- precedes *m*-; *e.g.*, *cyclo*hexyl is arranged under h, *iso*propyl under p, *n*-propyl under p, *allo*cholesteryl under c. The order for isomers is, *e.g.*, *n*-butyl, *iso*butyl, *sec.*-butyl, *tert.*-butyl, and *o*-chlorophenyl, *m*-chlorophenyl, *p*-chlorophenyl.

(*l*) Use of the alphabetical order does not affect the rule that one functional group, if present, should normally be cited as a suffix; *e.g.*,

2-chloro-3-methyl*cyclo*hexane-1-carboxylic acid

(*m*) Exceptions may be made when *essential* for clarity (*e.g.*, methylchloroarsine) or when the name of a substituent has become merged into that of another grouping so as to form virtually a trivial name (*e.g.*, propylnitramine).

(*n*) Differences from American practice (cf. above) are exemplified by **diphenylyl** (not biphenylyl), ***iso*propyl** (not isopropyl), ***iso*oxazolyl** (not isoxazolyl), **g**lyoxalinyl (not imidazolyl), **k**eto (not oxo).

Optically Active Isomers.—Small capital letters, D-, L-, and DL-, as agreed internationally, are used for optically active compounds which can be correlated sterically with glyceraldehyde or serine (see Mitchell, *op. cit.*, pp. 74, 84). In *all* other cases (+)-, (−)-, (±)-, or (without hyphens) *dextro*, *lævo*, and (optically) inactive are used.

Crombie and Harper (*J.*, 1950, 2687) have proposed D_a-, L_a- as prefixes for asymmetry which can be correlated with that of 2-methylbutanol, but Linstead *et al.* (*J.*, 1950, 3331, 3333) used the less definite forms *D*-, *L*- for the same purpose.

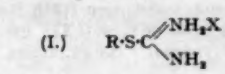
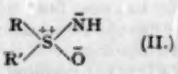
Cations.—Nitronium, NO_2^+, and nitrosonium, NO^+, have long been used. More recently, cations consisting of a positively charged organic radical have been named by adding "ium" to the name of the radical, *e.g.*, acetylium $CH_3{\cdot}CO^+$ (*J.*, 1950, 1203; 1949, 1452, 2034), benzoylium $Ph{\cdot}CO^+$ (*J.*, 1950, 2997), acylium $R{\cdot}CO^+$ (*J.*, 1950, 1447, 1460). Cations formed from neutral molecules by addition of a proton have been named by adding "ium" to the whole name of the substance, *e.g.*, nitric acidium $H_2^+NO_3$, acetic acidium $CH_3{\cdot}CO_2H_2^+$, acetic anhydridium $(CH_3{\cdot}CO)_2OH^+$ (*J.*, 1950, 1203).

Meso-ionic Compounds.—The term "meso-ionic" was coined by W. Baker (*J.*, 1949, 307), and its correct usage has been discussed by him in a later paper (*J.*, 1950, 1545) which should be consulted for details. Further examples are recorded by Brown and Hammick (*J.*, 1950, 628).

Aliphatic Carboxylic Acids.—After many years during which enumeration of the carbon atoms in aliphatic acids sometimes did, and sometimes did not, include the carbon atom of the carboxyl group, the following practice is now established: (i) The carboxyl-carbon atom carries the number 1 when the name used for the acid ends in anoic, enoic, ynoic, dienoic, etc. (Geneva Convention, 1892). (ii) Greek letters, with the carboxyl-carbon atom excluded, are used with trivial names. (iii) Names according with I.U.C. rule 29 may be used, whereby acids are named as hydrocarbon-carboxylic acids, the carboxyl-carbon atom not being numbered. (iv) Geneva numbering ($CO_2H = 1$) may be used for long-chain fatty acids called by trivial names, in accordance with custom. To avoid confusion with past British practice, abbreviated names such as decoic (in place of decanoic) acid are not used, and a footnote is added specifying the enumeration whenever doubt might arise. Examples are: $CH_3{\cdot}CHBr{\cdot}[CH_2]_3{\cdot}CO_2H$, 5-bromohexanoic * or 4-bromopentane-1-carboxylic acid; $CH_3{\cdot}CH{:}CH{\cdot}CH_2{\cdot}CO_2H$, pent-3-enoic acid * or but-2-ene-1-carboxylic acid; $CH_3{\cdot}CH_2{\cdot}CHBr{\cdot}CO_2H$, α-bromobutyric acid or 2-bromobutanoic acid *; $CH_3{\cdot}[CH_2]_7{\cdot}CH(OH){\cdot}CH(OH){\cdot}[CH_2]_7{\cdot}CO_2H$, 9 : 10-dihydroxystearic acid * or 8 : 9-dihydroxyheptadecane-1-carboxylic acid.

* Geneva numbering, $CO_2H = 1$.

Thiuronium Salts.—Salts of the general formula (I) have been termed *S*-substituted thiuronium or thiouronium salts, with or without *iso*- or *ψ*- as prefix. Of these variants, the simplest has now been adopted as the standard form (cf. *J.*, 1949, 1996; 1950, 115, 1207), in accordance with recent American practice.

(I.)  (II.) 

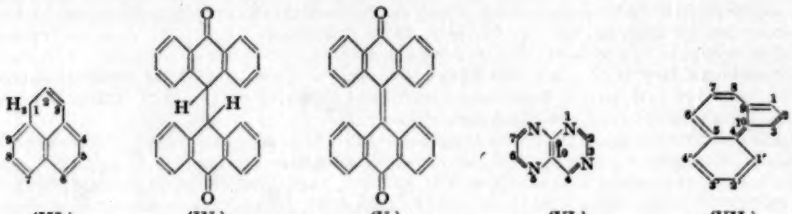
Thus, (I; R = CH_2Ph, X = Cl) is now called *S*-benzylthiuronium chloride. Elision of the "o" is not considered objectionable in this case as the derivation from thiourea is in any case irregular.

Sulphoximines.—This name has been adopted for compounds of type (II) (*J.*, 1950, 2081), as an abbreviated form of sulphoxidimine. The same name had been adopted in America, but for a different reason (personal communication from Dr. Patterson). The differing derivations lead to different names for somewhat similar types, and caution is needed in naming related types of compound if confusion is to be avoided; a common policy is being sought.

Nitramines, etc.—Nitramine (not nitroamine) is the name now used for compounds containing the grouping $>N{\cdot}NO_2$ (*J.*, 1950, 2657). It is regarded as a "trivial" name for a group which is complete in itself (as is, *e.g.*, benzamido), and the syllable "nitr" is not detached from "amine" when prefixes are arranged alphabetically (see p. 3700). The same applies to nitrosamine, bromamine, etc.

Perinaphthene.—This name and the numbering (III) have been adopted (cf. *J.*, 1949, 1768; Ring Index No. 2031).

Dianthronyl, etc.—The substance (IV), previously termed 9 : 9′- or 10 : 10′-dianthronyl, has been named dianthron-9-yl, and the substance (V), previously termed 9 : 9′-dianthraquinone, has been named dianthron-9-ylidene (*J.*, 1950, 2211, 2246).



(III.) (IV.) (V.) (VI.) (VII.)

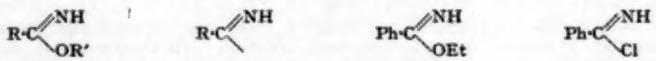
Pteridine.—Numbering as (VI) has been adopted for pteridine (cf. *J.*, 1949, 2003). This is the Ring Index method, augmented by numbering of the ring junctions as 9 and 10. For a further example of the numbering of ring junctions see 4 : 5-benzazulene (VII) (*J.*, 1950, 1352).

Sterols.—The conventions proposed by Fieser and Fieser (*Experientia*, 1948, **4**, 285) concerning the use of α, β, " α ", " β ", a, and b in the sterol series have been adopted (details are also given in *J.*, 1949, 1672). The adoption of further conventions in this field awaits the outcome of a conference organised by CIBA in the summer of 1950. Steric relations must always be indicated in full in structural formulæ of sterols.

Organosilicon Compounds.—For these, useful and comprehensive instructions have been provided by the International Union (15th Report, etc., pp. 127—132 *). By their use, compounds $R_3Si{\cdot}S{\cdot}SiR_3$ have been conveniently named as substituted disilthians (*J.*, 1950, 3077).

Suffixes.—Attention is drawn to I.U.C. rule 51 (*J.*, 1931, 1614), which prescribes that only one type of functional group may be expressed as suffix. For enumeration, the lowest available number is assigned to the suffix (I.U.C. rule 64). Breach of these rules has been very common, but they should always be strictly observed. Suffixes " ene " and " yne " are not considered as " functional " for the purpose of rule 51.

Imidic Acids.—Naming compounds of type (VIII) as imino-ethers (or imido-esters), and halides such as (XI) as imino-halides is fraught with difficulty in complex cases : either the hyphen is omitted, so that a word ends in " o ", or the hyphen is retained and the complete name is very hard to unravel. The American practice, whereby compounds (VIII; R′ = H) are



(VIII.) (IX.) (X.) (XI.)

termed imidic acids, has now been adopted by the International Union (15th Report, etc., p. 135, rule 58·8 *), as has the termination imidoyl for the radicals of type (IX); use of this much more convenient terminology will be encouraged in the *Journal*. As examples, (X) is ethyl benzimidate, and (XI) is benzimidoyl chloride.

Unsaturated Compounds.—When a numerical significance attaches to a termination " ene " or " yne," the position of the unsaturation is indicated by numerals placed immediately in front of these syllables, *e.g.*, hex-1-ene, hexa-1 : 5-dien-3-yne, *cyclo*hex-3-ene, cholest-4-ene (contrast indene, xanthen) (cf. Mitchell, *op. cit.*, pp. 42, 44). The degree of reduction of aromatic compounds is normally indicated by enumerating the reduced positions, *e.g.*, 1 : 4-dihydronaphthalene. However, for almost completely reduced compounds use of the Greek capital Δ is convenient, as in Δ^9-octahydronaphthalene; and this symbol is also sometimes useful when terminations indicating partial reduction are used, as in Δ^2-thiazoline (*J.*, 1950, 1899), Δ^3-pyrroline (cf. also *J.*, 1950, 3591).

Methyl-substituted Benzene Derivatives.—In all names derived from toluene or xylene the lowest numbers are assigned to the methyl groups (Mitchell, *op. cit.*, p. 113). Thus, (XII) is 4-nitro-*o*-toluic acid, (XIII) is 5-chloro-*o*-4-xylenol, and the radical (XIV) is 2-chloro-*p*-tolyl. This is peculiar to British nomenclature, and it is restricted to methyl-substituted compounds

* Consideration of the remainder of the recommendations on organic nomenclature is deferred.

as, *e.g.*, (XV) is 2-ethyl-5-nitrobenzoic acid (contrast XII). It is strongly recommended that complex benzene derivatives should be named as methyl-substituted benzene derivatives, *e.g.*, (XIII) as 2-chloro-4 : 5-dimethylphenol.

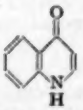
(XII.)

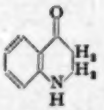
(XIII.)

(XIV.)

(XV.)

Heterocyclic Ketones.—Names such as 4-quinolone (XVI) for heterocyclic ketones are well-established. It therefore appears that the further-reduced compounds should be named on the pattern of 2 : 3-dihydro-4-quinolone for (XVII); but this obscures the true state of reduction,

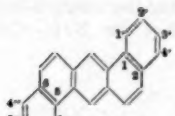
(XVI.) 



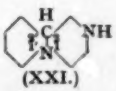
(XVII.)

e.g., in (XVII) two of the double bonds of quinoline have been removed; such reduced heterocyclic ketones are therefore best named by means of keto- and hydro-prefixes, *e.g.*, (XVII) is 1 : 2 : 3 : 4-tetrahydro-4-ketoquinoline.

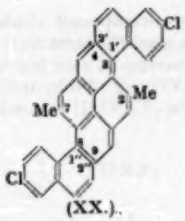
Polycyclic Compounds.—As is well known, the general British practice for compounds containing fused rings is in line with that used in Beilstein, but certain features are not always appreciated. The name for the whole system is built up from those of the component ring systems, and the original numbering of the components is retained in the numbering of the compound system. Examples of the typographical style now adopted in the *Journal* are 1 : 2-benzanthracene, 1 : 2-5 : 6-dibenzanthracene (XVIII), thiopheno(3′ : 2′-2 : 3)pyrrole (XIX), 6′ : 6″-dichloro-2 : 7-dimethyldinaphtho(1′ : 2′-3 : 4){1″ : 2″-8 : 9)pyrene (XX), and piperidino-(1′ : 2′-1 : 2)piperazine (XXI).


(XVIII.)

(XIX.)



(XXI.)



(XX.)

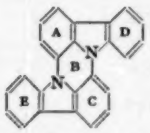
These examples illustrate also the assignment, to the ring junctions, of the lowest numbers available from the standard numbering of the component rings (substituents are neglected for this purpose), and also the numbering of added benzene rings outwards starting from the unnumbered carbon atom next to that carrying the lower number of the main component. Some of the many further examples are to be found in *J.*, 1949, 670, 2013; 1950, 344, 607, 680, 1114, 1147.

The letter " o," as in furano, indeno, etc., is used at the end of the first-named ring-system to denote ring union. Terminations as in naphtha or phenanthra are now restricted to the quinones and the like. Added benzene rings are denoted by " benzo," but the " o " of " benzo " is elided before a vowel, as in benzanthracene, and in past British practice also before a consonant when euphony appears to make this preferable (cf. benzpyran, benzfuran); the Ring Index and *Chemical Abstracts* permit elision only before a vowel. As personal ideas of euphony vary and as the elision markedly affects indexing, the American practice will in future be encouraged in Chemical Society publications.

In some complex cases the British system becomes unwieldy, and Ring Index names and numbering, if simpler, may then be used, either as sole names or as alternatives in parentheses.

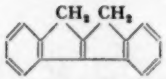
Occasionally a symmetrical structure is most simply named from diradical components. For instance, (XXIIa), which was conveniently termed 1 : 9-9′ : 1′-dicarbazolylene (*J.*, 1950, 2120),

would be harder to name in any other way [*e.g.*, 5 : 10-dihydro-1 : 10-5 : 6-di-*o*-phenylenephenazine—cf. (XXII*a*) written as (XXII*b*)].

(XXII*a*.) 

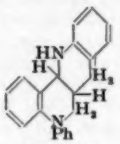
(XXII*b*.)

The state of reduction of fused rings sometimes requires careful interpretation. For example, according to British practice, (XXIII) is indeno(2′ : 3′-2 : 3)indene, because the CH_2 groups are each present in the indene components; the substance (XXIV) would be 1 : 1′-dehydro-

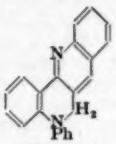
(XXIII.) 

(XXIV.)

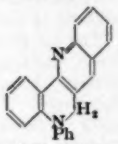
indeno(2′ : 3′-2 : 3)indene; this contrasts with the Ring Index, where (XXIV), being the least hydrogenated form possible, is given the fundamental name indeno[1, 2-*a*]indene (R.I. 2321), and (XXIII) would be a dihydro-compound. Another type of case in which care is required is exemplified by (XXV), where union of two tetrahydroquinoline rings gives 1 : 2 : 3 : 4 : 1′ : 4′-*hexa*hydro-1-phenylquinolino(3′ : 2′-3 : 4)quinoline (*J.*, 1949, 2817); (XXVI*a* = *b*) is the



(XXV.)



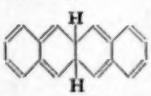
(XXVI*a*.)



(XXVI*b*.)

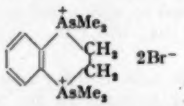
dihydro-compound although the left-hand quinoline system appears to be in the tetrahydro-state when the formula is written as (XXVI*a*). Even greater care is required when hetero-atoms are present at ring junctions. Thus, the simplest method of recognising the dihydro-state of (XXVII) [2 : 3-dihydrophthalazino(2′ : 3′-2 : 3)phthalazine] is to replace the N by CH, to obtain (XXVIII) (in analogous cases, O or S must replaced by CH_2).

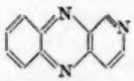
(XXVII.)



(XXVIII.)

"Oxa-aza" Convention.—The "oxa-aza" convention for naming heterocyclic compounds is well-known (I.U.C. rule 16; Mitchell, *op. cit.*, pp. 97, 106). It is not at once applicable when the hetero-atom also requires functional designation, as do the arsonium atoms in (XXIX);

(XXIX.) 



(XXX.)

this compound was termed 1 : 2 : 3 : 4-tetrahydro-1 : 1 : 4 : 4-tetramethyl-1 : 4-diarsonianaphthalene dibromide (*J.*, 1950, 683), and this name seems readily intelligible although arsonia (in contrast to arsa) is not a "recognised" prefix (the name, 1 : 1 : 4 : 4-tetramethyl-*o*-phenyleneethylenediarsonium dibromide, was also given as an alternative).

It is not always realised that the "oxa-aza" convention must not be applied to the name of a heterocyclic system; one must go right back to the parent hydrocarbon. For instance, if named by this convention, (XXX) must be 2 : 9 : 10-triaza-anthracene (*J.*, 1949, 2540); names such as 2-azaphenazine or 5 : 8-diaza-6 : 7-benz*iso*quinoline may appear attractive to provide analogies with other systems discussed in a particular paper but multiply the alternatives excessively.

Typographical.—There has in the past been no consistency in the use of parentheses when naming substituents which are themselves substituted. The following principles have been adopted, as a "house custom," being designed to combine clarity with the minimum of symbols. Parentheses are not used when only one numeral or positional letter follows the main positional indication, as in 1-2′-aminoethylpyridine, 2-α-hydroxybenzylpyridine, *o*-2-aminoethylaniline, 2-*o*-aminophenylethylamine. When more than one positional indication is required for substituents in the substituent, parentheses are used, as in *o*-(2 : 2 : 2-trichloroethyl)phenol, 1-(2-chloro-4-nitrophenyl)anthracene, 1-(3 : 4-dimethoxyphenyl)anthracene. Numerals are not primed (*i.e.*, 3, not 3′) inside parentheses, as the parentheses remove the need for this distinguishing mark. These general principles may be modified when clarity demands it.

Acknowledgment is gratefully made to the many authors who have given the Editors the benefit of their specialist knowledge in some of the above and numerous other fields. Finally, it is with great pleasure that we record our thanks to American colleagues, notably Drs. A. M. Patterson, E. J. Crane, and H. S. Nutting, for much help from their long and wide experience; the large correspondence has ranged over a very wide field with the object, which it is believed will be gradually achieved, of largely diminishing the present, and preventing future, divergences between American and British nomenclature, to the advantage of all chemists.

[*December 11th*, 1950.]

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